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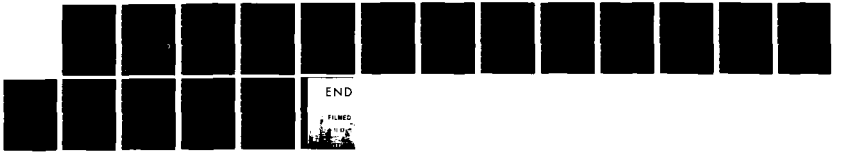

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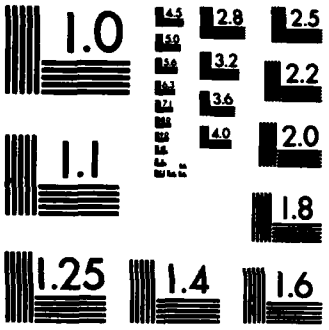

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Three established computer codes that are used in the calculation of equilibrium composition of combustion products are reviewed and recommendations made concerning their utilization in detonation problems with dispersed explosives.

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A Computer Study of Detonation Waves in Dispersed Powdered High Explosives

Final Report

AFOSR-81-0230

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I. INTRODUCTION

When a chemical reaction takes place old chemical bonds are broken and new ones formed. The energy associated with these bonds either appears in the form of heat or results in the absorption of heat from the surroundings. A rapid exothermic reaction in which some of the reactants are oxidized is known as a combustion reaction. The zone in which combustion reactions take place is known as the reaction zone and as it moves relative to an unburned mixture it is known as a combustion wave.

A detonation wave is a special case of the combustion wave in that it moves with a supersonic velocity relative to the unburned mixture and it is sustained by the energy liberated in the chemical reaction. It is composed of a shock wave, or discontinuity, which propagates into an explosive material, compressing and heating it, thus triggering chemical reaction. A balance is achieved such that the chemcial reaction then supports the shock.

Detonation waves have been studied extensively from both experimental and theoretical points of view for several years. Considerable work has been done on the detonation of explosives that exist in the gaseous, liquid, or condensed solid state. On the other hand, a limited amount of attention has been given to the study of a cloud of powdered explosive dispersed in air.

II. THEORETICAL DESCRIPTION

After initiation, the detonation will reach a steady state in which it propagates into an unreacted mixture at a constant supersonic velocity. In order to predict the pressures generated by such a wave, among other things, it is necessary to formulate the phenomenon analytically as was first done by D. Chapman and E. Jouget around 1900. Results of their work, known as CJ theory, are still utilized extensively today.

A. Chapman - Jouget Theory

The assumptions made in order to formulate the CJ model of a detonation wave are as follows:

1. The flow is one-dimensional and laminar.

2. The detonation wave is pictured as a jump discontinuity, a shock across which the basic conservation laws apply. The chemical reaction is regarded as instantaneous so that there is essentially no reaction zone, only a region in which the unburned mixture exists in thermodynamic equilibrium and a region in which the gaseous products of reaction exist (also in thermodynamic equilibrium), the regions separated by the shock.

3. The motion of the detonation as it moves into the explosive is independent of time. (Steady)

B. Basic Conservation Laws

If we consider a detonation wave moving with a velocity D into an explosive initially at rest then the basic conservation laws, when applied to such a system, result in the following equations.

Conservation of Mass: $$\rho_0 D = \rho(D-U) \tag{1}$$

where ρ_0 = density of the unreacted explosive (initial state)

ρ = density of the gaseous product mixture (final state)

U = velocity of the gaseous products

Conservation of Momentum: $$p_0 + \rho_0 D^2 = p + \rho(D-U)^2 \tag{2}$$

where p_0 = pressure of initial state

p = pressure of final state

Conservation of Energy: $$E + \frac{p}{\rho} + \frac{1}{2}(D-U)^2 = E_0 + \frac{p_0}{\rho_0} + \frac{1}{2} D^2 \tag{3}$$

where E = specific internal energy

Equation of State: $$E = E(p,\rho) \tag{4}$$

For an ideal gas

$$E - E_0 = C_v T - C_{vo} T_0 - q = \frac{p}{\rho}\left(\frac{1}{\gamma-1}\right) - \frac{p_0}{\rho_0}\left(\frac{1}{\gamma-1}\right) - q$$

where C_v = constant volume heat capacity

q = heat of reaction

γ = ratio of specific heats

We have therefore a system of four equations in the five unknowns ρ, U, D, p, and q. Further assumptions must therefore be made in order to ascertain state of the reaction products following the detonation.

C. Determination of the CJ Detonation Velocity

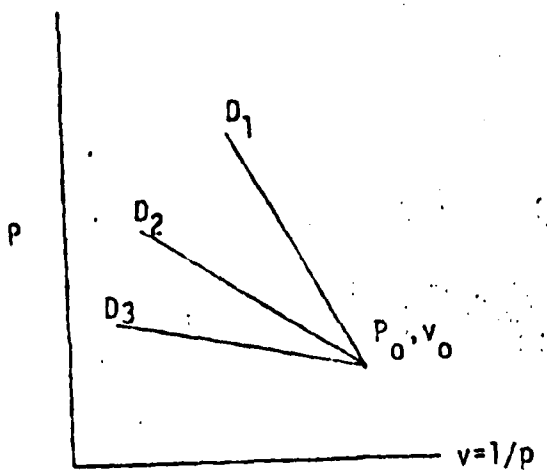
If U is eliminated from Eqs. (1) and (2), one obtains an equation that may be plotted as a line in the p-v ($v=1/\rho$) plane and is known as a Rayleigh line. This line shows the variation of product pressure and specific volume for particular detonation velocities. (Fig. 1a)

If U and D are eliminated from Eqn. (3) via Eqns (1) and (2), one obtains an equation that may be plotted in the p-v plane and is known as a Hugoniot curve. This gives the volume as a function of internal energy, E (p,v), which is given as an equation of state. (Fig. 1b)

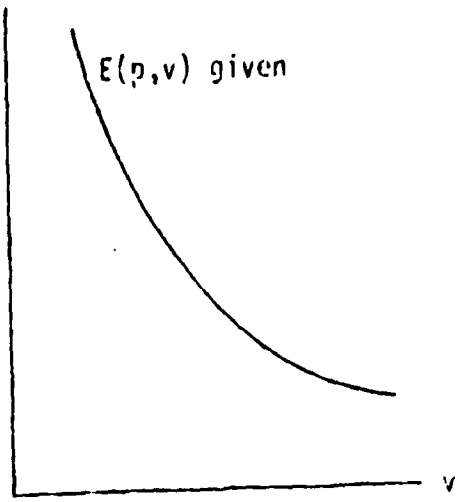
The state (p,v) of the reacted products may than be determined, for a given detonation velocity, as the intersection of the Rayleigh line and Hugoniot curve. (Fig. 1c)

The expression for the Rayleigh line contains the detonation velocity as a parameter so the entire family of Rayleigh lines should be considered, three of which are shown in Fig. 1c.

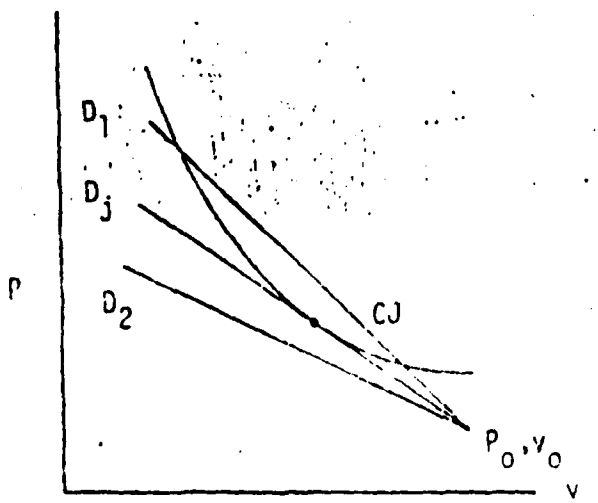
For a sufficiently small detonation velocity, say D_2, the two curves do not intersect so there is no solution. For a large value, D_1, there are two solutions, denoted S (strong) and W (weak). And for a particular value of D, D_j, there is one unique solution. The Chapman - Jouguet hypothesis is that the steady detonation velocity is indeed this value, i.e., the minimum velocity consistent with the conservation equations. Other solutions, for $D>D_j$ are



1a. Rayleigh lines



1b. Hugoniot curve



1c. Hugoniot and Rayleigh curves

Figure 1 Rayleigh - Hugoniot Curves

rejected because of physical reasonings.

D. Solution of Governing Equations Under the CJ Hypothesis

The CJ hypothesis may be used together with one further assumption in order to obtain a very simple system of governing equations. This assumption is essentially that the detonation wave is a "strong" reaction or disturbance. In other words, one might also say that the Mach number of the detonation wave is large or that the pressure change resulting from the passage of the detonation wave is large. If such is the case then the system of governing equations may be reduced to

$$\rho = \rho_0 \left(\frac{\gamma}{\gamma+1} \right) \qquad p = \frac{\rho_0 D^2}{\gamma+1} \qquad D^2 = 2(\gamma^2-1)q \tag{5}$$

If, therefore, the density of the initial explosive, the heat of reaction, and the product ratio of specific heats are known, the CJ pressure, density, and detonation velocity may be determined. It is, however, a rather formidable task to compute the equilibrium composition of the combustion products (which is necessary to obtain γ for example), and this is almost always handled by means of established computer codes.

III. PURPOSE OF RESEARCH

Two groups have been involved in theoretical/experimental work on the problem of the detonation of dispersed high explosives: The Gas Dynamics Laboratory at the University of Michigan [6] and the Illinois Institute of Technology Research Institute (IITRI) [9]. Both groups utilize the CJ detonation model to theoretically predict the pressures and other flow variables. The governing equations, Eqs. (5), indicate that it is the composition of the products of combustion that influence the CJ pressure, detonation velocity, etc. It is therefore necessary to determine the equilibrium state of the combustion products. The Michigan group utilizes the Gordon-McBride [4] computer program to do so, whereas IITRI uses their own EQUIL code [8].

It is the purpose of this report to discuss three established computer codes that are used in the calculation of equilibrium composition of combustion products, namely:

A. Gordon and McBride's program as described in NASA SP-273,

B. EQUIL program, written by IITRI, and

C. TIGER, written by Ballistic Research Laboratories [2].

IV. DESCRIPTION OF COMPUTER CODES

A. Gordon and McBride [4].

The Gordon-McBride code is a well-accepted and readily available code that can be utilized to calculate equilibrium compositions for CJ

detonations. The program combines the thermodynamic equilibrium calculations and the CJ Equations (Eqs. (5)) to completely define the detonation wave. The condition for equilibrium may be stated in terms of any of several thermodynamic functions such as the free energy or entropy. This treatment iteratively minimizes the free energy to calculate the equilibrium composition and properties of perfect gas mixtures.

There are three steps in the calculation of the CJ parameters. First an initial estimate is made of the detonation pressure and temperature. Then an improved estimate is obtained via a recursion formula and finally the correct values evaluated by a Newton-Raphson iteration procedure.

The input specifies the fuel and oxidizer composition, enthalpy, density, and the equivalence ratio. The output includes properties of the burned and unburned gases, detonation velocity, detaonation ratios P/Po, T/To, ρ/ρ_0, and the final equilibrium composition.

B. EQUIL [8].

The computer program EQUIL was written by Dr. R. Snow for IITRI and is "proprietary material" and not obtainable, hence thepresent discussion is based solely on information supplied by that contractor.

It can be shown that if P_v = pressure reached in a constant volume explosion then $P_{cj} = 2P_v$. The IITRI EQUIL computer program is based on

the minimization of Gibb's free energy, which should be done under the constraint of constant temperature. By using various heat balances, however, the program computes the pressure, not at constant temperature but at constant volume, and then relates this value to the CJ pressure through the above relationship.

C. TIGER [2].

TIGER is a highly complex computer code designed to calculate detonation properties under a wide variety of thermodynamic conditions, for example, utilizing different equations of state. The four volume documentation listed in the bibliography includes theoretical discussions and will be referenced here rather than discussed in detail.

V. CONCLUSIONS AND RECOMMENDATIONS

All three computer programs are dependent upon thermodynamic data as input for their calculations. The acquisition of acceptable data for explosive compounds is a major task in itself and numerous sources are presently available (for example see Refs. (1), (3), (7)). Conflicting values are present in almost all sets, and there are numerous arguments in the current literature as to why one version is superior to another. The JANAF tables [4] have long served as a standard and, outside of that source, it is difficult to obtain values for S^0 for example.

Using the JANAF tables, one can run the Gordon-McBride program for

various fuel/oxidants and initial conditions. A typical output is attached. This program is well-documented, [4], easily run, and although limited to perfect gases, gives feasible results that could provide a starting point, should further refinements become necessary.

The EQUIL program, since it is proprietary in nature, cannot be obtained and one must rely on IITRI and the corresponding interpretation of results. This has been done with confidence in the past [9], and it is felt that the two programs will give results that, although not in exact agreement by any means, differ by an acceptable amount, if corresponding thermodynamic data are used. It, also, is limited to the case of perfect gases.

TIGER, written in FORTRAN IV, is an immense program that is neither user-friendly nor system-friendly. Large amounts of man-hours and computer funds were expended and no acceptable results obtained. It supposedly has the capability of providing various equations of state and many other refinements, yet is a code that the somewhat-casual user should approach with extreme caution.

In conclusion, as one seeks to numerically determine the equilibrium composition of combustion products, one must first have acceptable thermodynamic data, regardless of which code is used, since each and every code is highly dependent upon such data. Gordon and McBride offer a readily available, user-friendly code that produces results which, although limited in many ways, provide an excellent first plateau. For many applications no further refinements would be

necessary. The EQUIL program is greatly limited because of its availability although results obtained from that program have proved satisfactory when compared with experiment [9]. The TIGER program offers the highest degree of flexibility and power, but one must be intimately associated with the problem under consideration and the code itself in order to avail oneself of such power.

Bibliography

1. Baer and Bryson, "Tables of Computed Thermodynamic Properties of Military Gun Propellants", BRL Memorandum Report No. 1338, March 1961.

2. Brinkley, et al., "TIGER Computer Program Documentation", Ballistics Research Laboratories, Aberdeen, MD, Nov. 1968.

3. Fedoroff and Sheffield, "Encyclopedia of Explosives and Related Items", Picatinny Arsenal, Dover, NJ, 1962.

4. Gordon, S. and McBride, B. J., "Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shocks, and Chapman-Jouguet Detonations", NASA SP-273, 1971.

5. "JANAF Thermochemical Tables", Dow Chemical Company, Midland, MI, Dec. 1960.

6. Kauffman, C. W., et al., "Detonation Characteristics of Dusts Dispersed in Air", Annual Rept. U. of MI., UM-016968, June, 1980.

7. "Properties of Explosives of Military Interest", AMC Pamphlet, AMCP 706-177, March 1967.

8. Snow, R., "Computer Procedures for Determining Chemical Equilibrium", IITRI Rept. C929-3, 1963.

9. Tulis, A. J., Austing, J. J. and Sumida, W. K., "Cane Tip Parameter Study", IITRI Phase I Tech. Rept., Jan. 1980.

ATTACHMENT

DETONATION PROPERTIES OF AN IDEAL REACTING GAS

CASE NO. 1

	CHEMICAL FORMULA							WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
OXIDANT	O	2.00000						1.00000	0.0	G	298.15	0.0
FUEL	C	3.00000	H	6.00000	C	6.00000	N	6.00000	1.00000	14710.000	G	298.15	0.0

O/F= 0.8644 PERCENT FUEL= 53.6373 EQUIVALENCE RATIO= 0.5000 REACTANT DENSITY= 0.0

UNBURNED GAS

P1,ATM	1.0000
T1,DEG K	298.15
H1,CAL/G	35.52
M1,MOL WT	59.159

BURNED GAS

P, ATM	45.569
T, DEG K	3495
RHO, G/CC	4.4986-3
h, CAL/G	378.7
S, CAL/(G)(K)	2.3034
M, MOL WT	28.314
(DLV/DLP)T	-1.03080
(DLV/DLT)P	1.5647
CP, CAL/(G)(K)	1.1375
GAMMA (S)	1.1367
SON VEL,M/SEC	1080.1

DETONATION PARAMETERS

P/P1	45.569
T/T1	11.723
M/M1	0.4786
RHO/RHO1	1.8604
DET VEL,M/SEC	2009.5

FROZEN FRACTIONS

[illegible]	[illegible]
CO2	0.14385
H	0.00790
HNO	0.00001
HO2	0.00023
H2	0.00943
H2O	0.15811
H2O2	0.00002
N	0.00001
NO	0.04618
NO2	0.00011
N2	0.18104
N2O	0.00001

C	0.03823
CH	0.06895
O2	0.28472

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.50000E-05 FOR ALL ASSIGNED CONDITIONS

C(S)	C-	CH-	CH2	CH2O	CH3	CH4	CN	CNN	CN2
C2	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2O	C3	C3O2
C4	C5	HCN	HCO	HNCO	HNO2	HNO3	H2O(S)	H2O(L)	NCO
NH	NH2	NH3	NO3	N2H4	N2O4	N2O5	N3	O3	

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

CF = 0.648280

	EFFECTIVE FUEL	EFFECTIVE OXIDANT	MIXTURE
ENTHALPY	HPP(2)	HPP(1)	HSUBO
(KG-MOL)(DEG K)/KG	0.33326904E+02	0.0	0.20219208E+02

KG-ATOMS/KG	BOP(I,2)	BOP(I,1)	BO(I)
O	0.27012687E-01	0.62502325E-01	0.40970996E-01
C	0.13506342E-01	0.0	0.81942044E-02
H	0.27012687E-01	0.0	0.16388416E-01
N	0.27012687E-01	0.0	0.16388416E-01